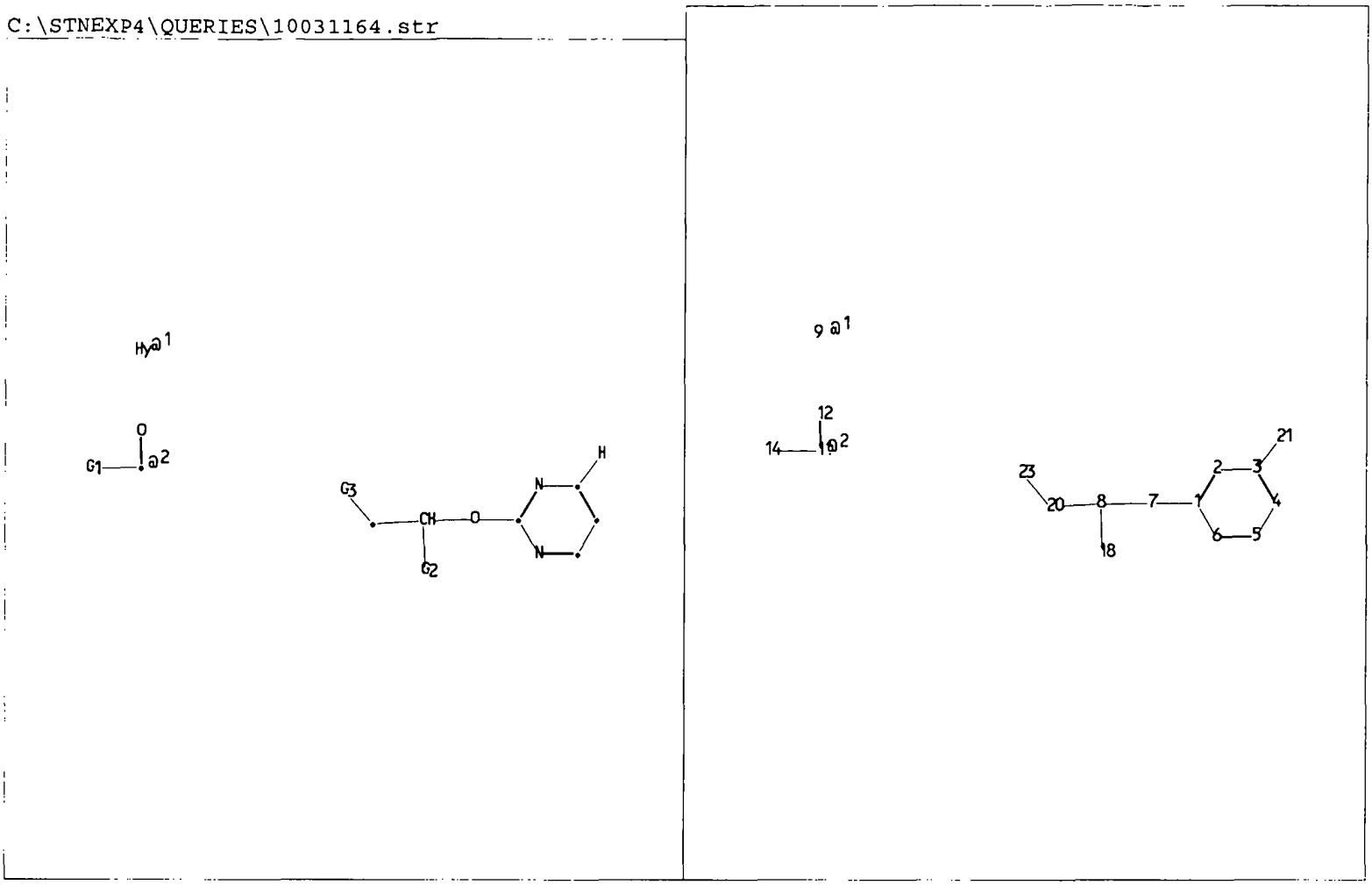
L Number	Hits	Search Text	DB	Time stamp
1	3690	((544/245) or (544/265) or (544/276) or (544/277) or (544/315) or (544/316) or (544/317) or (544/318) or (514/258.1) or (514/263.3) or (514/274)).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/12/01 11:45

C:\STNEXP4\QUERIES\10031164.str



chain nodes :
7 8 9 11 12 14 18 21 23
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
20
chain bonds :
1-7 3-21 7-8 8-18 8-20 11-12 11-14 20-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-7 7-8 8-18 11-12 11-14 20-23
exact bonds :
3-21 8-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,N,Hy

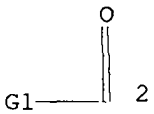
G2:[*1],[*2]

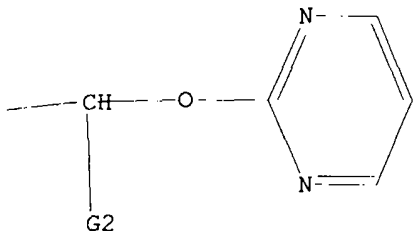
G3:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 11:CLASS
12:CLASS 14:CLASS 18:CLASS 20:CLASS 21:CLASS 23:CLASS
Generic attributes :
9:
Saturation : Unsaturated

```
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : 2 or more
    Type of Ring System    : Monocyclic

Element Count :
    Node 9: Limited
        C,C1
        N,N4
        O,O0
        S,S0
```

```
=>
Uploading 10031164.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1               STR

      Hy 1
```






```
G1 O,N,Hy
G2 [@1],[@2]


Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 12:45:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1346 TO ITERATE

 74.3% PROCESSED    1000 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        24720 TO    29120
PROJECTED ANSWERS:            1394 TO     2590

L2           50 SEA SSS SAM L1

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
```

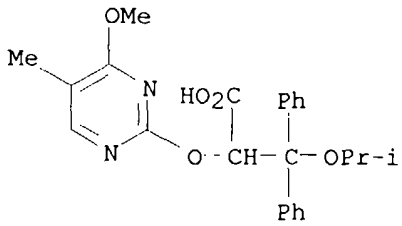
```
L3    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10031164.str

L4      STRUCTURE UPLOADED

=> que L4 NOT L3

L5   QUE L4 NOT L3

=> d l5
L5 HAS NO ANSWERS
L3              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L4              STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L5              QUE  L4 NOT L3


=> s l5 sss sam
SAMPLE SEARCH INITIATED 12:50:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    227 TO ITERATE

100.0% PROCESSED     227 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3637 TO     5443
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L4 NOT L3

=>
Uploading 10031164.str

L7      STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7              STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l7 sss sam
SAMPLE SEARCH INITIATED 12:50:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    237 TO ITERATE

100.0% PROCESSED     237 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          3817 TO     5663
PROJECTED ANSWERS:                0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 sss ful
FULL SEARCH INITIATED 12:50:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   4185 TO ITERATE

100.0% PROCESSED    4185 ITERATIONS                                 11 ANSWERS
SEARCH TIME: 00.00.01

L9            11 SEA SSS FUL L7

=> s l9
L10            3 L9

=> d l10 1-3 bib,ab,hitstr
```

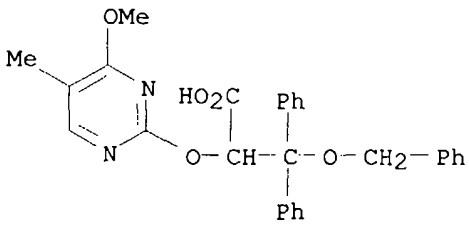
L10 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:63980 CAPLUS
DN 134:131546
TI Preparation of pyrimidinyloxypropionates as endothelin receptor antagonists.
IN Amberg, Wilhelm; Kettschau, Georg
PA Basf Aktiengesellschaft, Germany
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005771	A1	20010125	WO 2000-EP6293	20000705
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19933164	A1	20010125	DE 1999-19933164	19990720
	EP 1196394	A1	20020417	EP 2000-953009	20000705
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012592	A	20020528	BR 2000-12592	20000705
	ZA 2002000333	A	20030217	ZA 2002-333	20020115
	NO 2002000254	A	20020220	NO 2002-254	20020117
	BG 106321	A	20020830	BG 2002-106321	20020118
PRAI	DE 1999-19933164	A	19990720		
	WO 2000-EP6293	W	20000705		

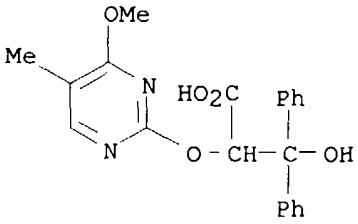
OS MARPAT 134:131546
AB Title compds. [I; R = tetrazolyl, acyl; R2 = OH, amino, alkyl, alkenyl, alkynyl, hydroxyalkyl, alkylthio, etc.; R3 = OH, amino, halo, alkyl, alkenyl, alkynyl, alkenyloxy, haloalkyl, alkoxy, haloalkoxy, alkylthio, etc.; R2R3 = atoms to form a 5-6 membered ring; R4, R5 = (substituted) Ph, naphthyl, cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, Ph, naphthyl, heteroaryl; Z = O, S], were prepd. Thus, a suspension of NaH in DMF at 0.degree. was treated with (S)-2-hydroxy-3-methoxy-3,3-diphenylpropionic acid in DMF and then with 2-methylsulfonyl-4-methoxy-5-methylpyrimidine (prepn. given) in DMF followed by stirring overnight to give (S)-2-(4-methoxy-5-methylpyrimidin-2-yloxy)-3-methoxy-3,3-diphenylpropionic acid. The latter showed Ki = 0.6 nM for binding to ETA receptors.
IT **321655-48-5P 321655-49-6P 321655-50-9P**
321655-51-0P 321655-52-1P 321655-54-3P
321655-55-4P 321655-59-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidinyloxypropionates as endothelin receptor antagonists)
RN 321655-48-5 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-(1-methylethoxy)-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 321655-49-6 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)

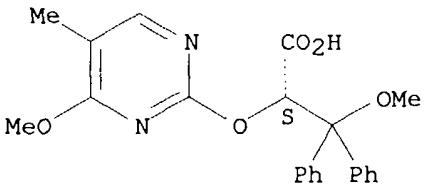


RN 321655-50-9 CAPLUS
CN Benzenepropanoic acid, .beta.-hydroxy-.alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl- (9CI) (CA INDEX NAME)



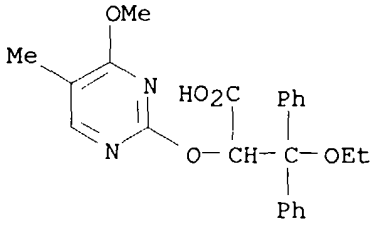
RN 321655-51-0 CAPLUS
CN Benzenepropanoic acid, .beta.-methoxy-.alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl-, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

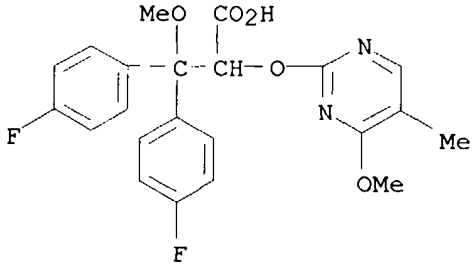


RN 321655-52-1 CAPLUS
CN Benzenepropanoic acid, .beta.-ethoxy-.alpha.-[(4-methoxy-5-methyl-2-

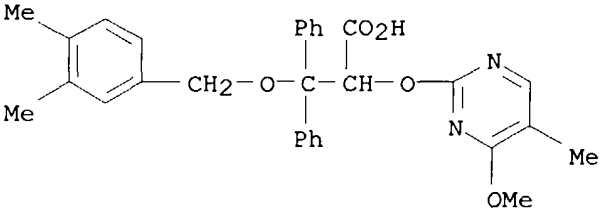
pyrimidinyl)oxy]-.beta.-phenyl- (9CI) (CA INDEX NAME)



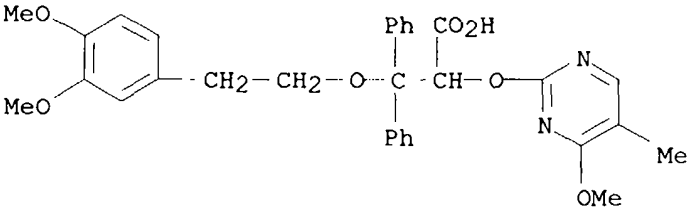
RN 321655-54-3 CAPLUS
CN Benzenepropanoic acid, 4-fluoro-.beta.-(4-fluorophenyl)-.beta.-methoxy-.alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]- (9CI) (CA INDEX NAME)



RN 321655-55-4 CAPLUS
CN Benzenepropanoic acid, .beta.-[(3,4-dimethylphenyl)methoxy]-.alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 321655-59-8 CAPLUS
CN Benzenepropanoic acid, .beta.-[2-(3,4-dimethoxyphenyl)ethoxy]-.alpha.-[(4-methoxy-5-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:538136 CAPLUS
DN 131:165311
TI New carboxylic acid derivatives with 5-substituted pyrimidine ring, their preparation and use as endothelin receptor antagonists
IN Amberg, Wilhelm; Jansen, Rolf; Kling, Andreas; Klinge, Dagmar; Riechers, Hartmut; Hergenroeder, Stefan; Raschack, Manfred; Unger, Liliane
PA BASF A.-G., Germany
SO Ger. Offen., 20 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19806438	A1	19990819	DE 1998-19806438	19980217
	CA 2321182	AA	19990826	CA 1999-2321182	19990205
	WO 9942453	A1	19990826	WO 1999-EP776	19990205
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9930271	A1	19990906	AU 1999-30271	19990205
	BR 9907911	A	20001024	BR 1999-7911	19990205
	EP 1066268	A1	20010110	EP 1999-911657	19990205
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	JP 2002503726	T2	20020205	JP 2000-532405	19990205
	ZA 9901214	A	20000816	ZA 1999-1214	19990216
	BG 104577	A	20010330	BG 2000-104577	20000704
	NO 2000004075	A	20000815	NO 2000-4075	20000815
	HR 2000000602	A1	20010630	HR 2000-602	20000913
PRAI	DE 1998-19806438	A	19980217		
	WO 1999-EP776	W	19990205		

OS MARPAT 131:165311
AB The title compds. [I; R1 = tetrazolyl, C(O)R; R = OR7, (substituted) N-linked 5-membered heteroarom. residue, O(CH2)pS(:O)kR8, NHSO2R9; R7 = H, cation, (substituted) C3-8 cycloalkyl, (substituted) C1-8 alkyl, (substituted) Ph, (substituted) CH2Ph, C3-6 (halo)alkenyl, C3-6 (halo)alkynyl; R8, R9 = (substituted) C1-4 alkyl, (substituted) C3-8 cycloalkyl, (substituted) C3-6 alkenyl, (substituted) C3-6 alkynyl, (substituted) Ph; k = 0-2; p = 1-4; R2, R3 = H, OH, (substituted) amino, halo, alkyl, alkenyl, alkynyl, hydroxyalkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph, (substituted) naphthyl, C3-7 cycloalkyl, etc.; R6 = H, (substituted) C1-8 alkyl, (substituted) C3-6 alkenyl, (substituted) C3-6 alkynyl, (substituted) C3-8 cycloalkyl, (substituted) Ph, (substituted) naphthyl, (substituted) 5- or 6-membered heteroarom. residue; X = halo, C1-4 haloalkyl, OH; Z = O, S, single bond], their enantiomers, diastereomers, and physiol. compatible salts are useful as endothelin receptor antagonists for treatment of diseases assocd. with elevated endothelin levels, such as chronic cardiac insufficiency, restenosis, hypertension, acute or chronic kidney failure, cerebral ischemia, asthma, benign prostate hyperplasia, and prostate cancer. Thus, Me 2-hydroxy-3-methoxy-3,3-diphenylpropionate reacted with NaH and 4,6-dimethoxy-5-fluoro-2-methylsulfonylpyrimidine in DMF to produce I (R1 = CO2Me, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = F, Z = O), which was sapond. to the corresponding acid (R1 = CO2H) (II). II bound to

endothelin ETA and ETB receptors with Ki 7.4 and 1200 nM, resp.

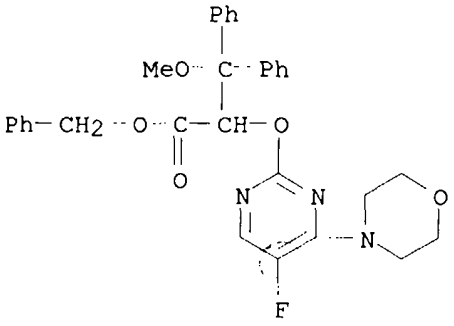
IT **238752-50-6P 238752-51-7P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(carboxylic acid derivs. with substituted pyrimidine ring, their prepn. and use as endothelin receptor antagonists)

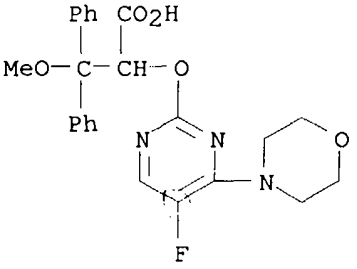
RN 238752-50-6 CAPLUS

CN Benzenepropanoic acid, .alpha.-[[5-fluoro-4-(4-morpholinyl)-2-pyrimidinyl]oxy]-.beta.-methoxy-.beta.-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



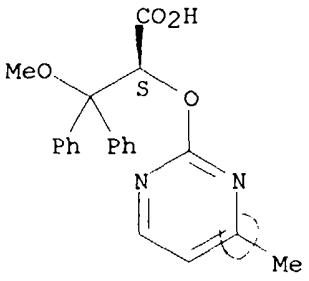
RN 238752-51-7 CAPLUS

CN Benzenepropanoic acid, .alpha.-[[5-fluoro-4-(4-morpholinyl)-2-pyrimidinyl]oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)



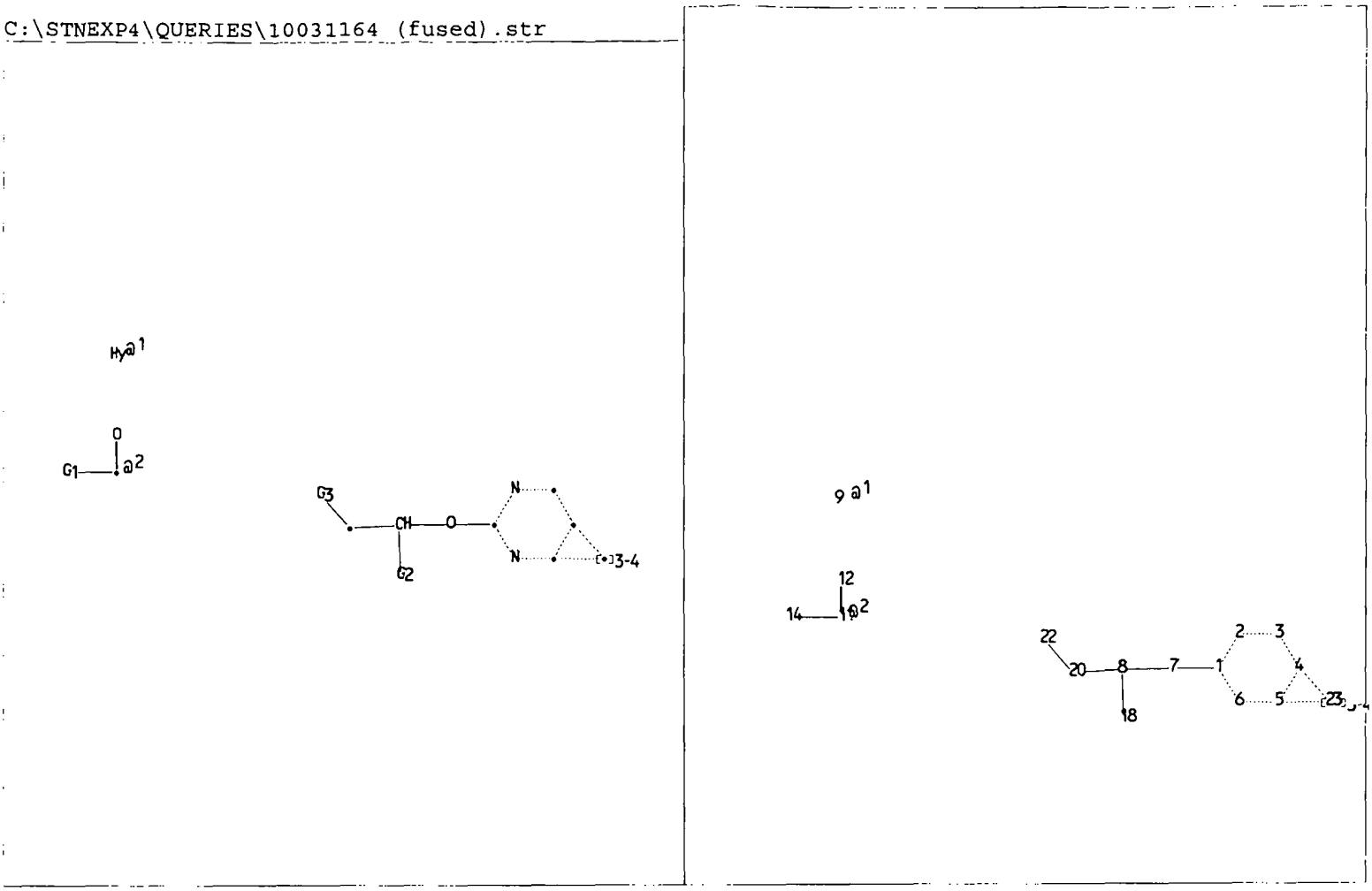
L10 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:271791 CAPLUS
DN 125:328
TI Discovery and Optimization of a Novel Class of Orally Active Nonpeptidic Endothelin-A Receptor Antagonists
AU Riechers, Hartmut; Albrecht, Hans-Peter; Amberg, Willi; Baumann, Ernst; Bernard, Harald; Boehm, Hans-Joachim; Klinge, Dagmar; Kling, Andreas; Mueller, Stefan; et al.
CS Hauptlaboratorium, BASF AG, Ludwigshafen, 67056, Germany
SO Journal of Medicinal Chemistry (1996), 39(11), 2123-8
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 125:328
AB A novel class of endothelin-A receptor ligands was discovered by high-throughput screening. Lead structure optimization led to highly potent antagonists which can be synthesized in a short sequence. The compds. are endothelin-A-selective, are orally available, and show a long duration of action.
IT **177036-97-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)
RN 177036-97-4 CAPLUS
CN Benzenepropanoic acid, .beta.-methoxy-.alpha.-[(4-methyl-2-pyrimidinyl)oxy]-.beta.-phenyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> d his

     (FILE 'HOME' ENTERED AT 12:44:52 ON 24 NOV 2003)

     FILE 'REGISTRY' ENTERED AT 12:44:57 ON 24 NOV 2003
L1             STRUCTURE UPLOADED
L2          50 S L1 SSS SAM
L3             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L4             STRUCTURE UPLOADED
L5             QUE L4 NOT L3
L6           0 S L5 SSS SAM
L7             STRUCTURE UPLOADED
L8           0 S L7 SSS SAM
L9          11 S L7 SSS FUL

     FILE 'CAPLUS' ENTERED AT 12:50:55 ON 24 NOV 2003
L10          3 S L9

     FILE 'CAOLD' ENTERED AT 12:51:15 ON 24 NOV 2003

=> s l9
L11          0 L9

=> log y
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                0.40     166.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -1.95

STN INTERNATIONAL LOGOFF AT 12:51:24 ON 24 NOV 2003
```

C:\STNEXP4\QUERIES\10031164 (fused).str



chain nodes :
7 8 9 11 12 14 18 22
ring nodes :
1 2 3 4 5 6 23
ring/chain nodes :
20
chain bonds :
1-7 7-8 8-18 8-20 11-12 11-14 20-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-23 5-6 5-23
exact/norm bonds :
1-2 1-6 1-7 2-3 3-4 4-5 4-23 5-6 5-23 7-8 8-18 11-12 11-14 20-22
exact bonds :
8-20

G1:O,N,Hy

G2:[*1],[*2]

G3:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 11:CLASS
12:CLASS 14:CLASS 18:CLASS 20:CLASS 22:CLASS 23:CLASS
Generic attributes :
9:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System : Monocyclic

Element Count :

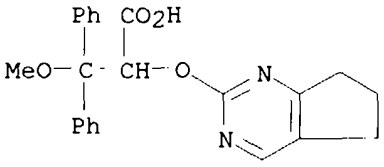
```
Node 9: Limited
    C,C1
    N,N4
    O,O0
    S,S0
```

```
=>
Uploading 10031164 (fused).str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:14:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     19 TO ITERATE

100.0% PROCESSED      19 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          119 TO      641
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss ful
FULL SEARCH INITIATED 10:14:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    445 TO ITERATE

100.0% PROCESSED     445 ITERATIONS                              17 ANSWERS
SEARCH TIME: 00.00.01

L3           17 SEA SSS FUL L1

=> s l3
L4            6 L3

=> d l4 1-6 bib,ab,hitstr
```

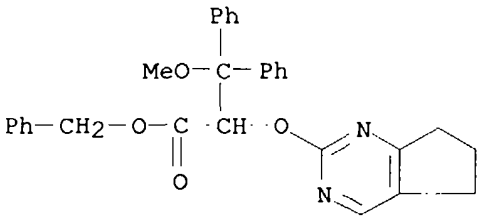
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:63980 CAPLUS
DN 134:131546
TI Preparation of pyrimidinyloxypropionates as endothelin receptor antagonists.
IN Amberg, Wilhelm; Kettschau, Georg
PA Basf Aktiengesellschaft, Germany
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005771	A1	20010125	WO 2000-EP6293	20000705
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19933164	A1	20010125	DE 1999-19933164	19990720
	EP 1196394	A1	20020417	EP 2000-953009	20000705
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012592	A	20020528	BR 2000-12592	20000705
	ZA 2002000333	A	20030217	ZA 2002-333	20020115
	NO 2002000254	A	20020220	NO 2002-254	20020117
	BG 106321	A	20020830	BG 2002-106321	20020118
PRAI	DE 1999-19933164	A	19990720		
	WO 2000-EP6293	W	20000705		

OS MARPAT 134:131546
AB Title compds. [I; R = tetrazolyl, acyl; R2 = OH, amino, alkyl, alkenyl, alkynyl, hydroxyalkyl, alkylthio, etc.; R3 = OH, amino, halo, alkyl, alkenyl, alkynyl, alkenyloxy, haloalkyl, alkoxy, haloalkoxy, alkylthio, etc.; R2R3 = atoms to form a 5-6 membered ring; R4, R5 = (substituted) Ph, naphthyl, cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, Ph, naphthyl, heteroaryl; Z = O, S], were prepd. Thus, a suspension of NaH in DMF at 0.degree. was treated with (S)-2-hydroxy-3-methoxy-3,3-diphenylpropionic acid in DMF and then with 2-methylsulfonyl-4-methoxy-5-methylpyrimidine (prepn. given) in DMF followed by stirring overnight to give (S)-2-(4-methoxy-5-methylpyrimidin-2-yloxy)-3-methoxy-3,3-diphenylpropionic acid. The latter showed Ki = 0.6 nM for binding to ETA receptors.
IT **321655-47-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidinyloxypropionates as endothelin receptor antagonists)
RN 321655-47-4 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)

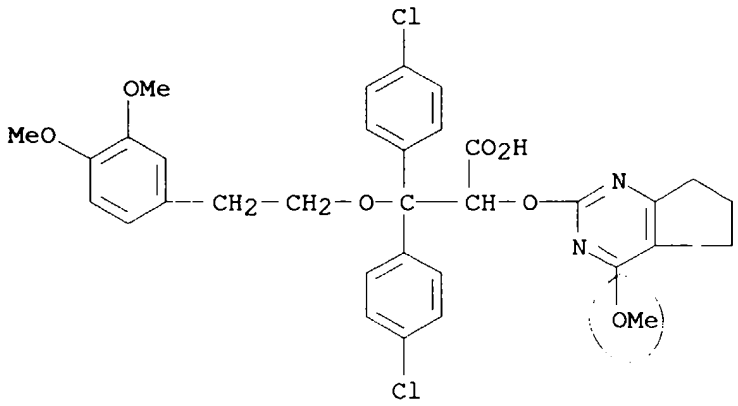


IT **321655-45-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyrimidinyloxypropionates as endothelin receptor antagonists)
RN 321655-45-2 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:455209 CAPLUS
DN 131:214248
TI Discovery and Synthesis of (S)-3-[2-(3,4-Dimethoxyphenyl)ethoxy]-2-(4,6-dimethylpyrimidin-2-yloxy)-3,3-diphenylpropionic Acid (LU 302872), a Novel Orally Active Mixed ETA/ETB Receptor Antagonist
AU Amberg, Willi; Hergenroeder, Stefan; Hillen, Heinz; Jansen, Rolf; Kettschau, Georg; Kling, Andreas; Klinge, Dagmar; Raschack, Manfred; Riechers, Hartmut; Unger, Liliane
CS Hauptlaboratorium, BASF AG, Ludwigshafen, 67056, Germany
SO Journal of Medicinal Chemistry (1999), 42(16), 3026-3032
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:214248
AB Structural variation of the endothelin A-selective antagonist I (R = Me; LU 135252) led to analogs which retain ETA affinity but exhibit substantial ETB affinity as well. Replacement of the .beta.-methoxy group of I (R = Me) with a more lipophilic side chain contg. a Ph group results in a substantial improvement in the ETB affinity, while the ETA affinity is retained. The most active deriv. obtained is I [R = 3,4-(MeO)2C6H3(CH2)2; LU 302872], which can be prepd. in enantiomerically pure form in eight steps via an acid-catalyzed transetherification. It has a Ki = 2.15 nM for binding to the ETA receptor and a Ki = 4.75 nM for binding to the ETB receptor, is orally available, and antagonizes the big ET-induced blood pressure increase in rats and the big ET-induced bronchospasm in guinea pigs, each time at a dose of 10 mg/kg.
IT **204267-56-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and SAR of mixed ETA/ETB receptor antagonist (dimethylpyrimidinyloxy)diphenylpropionic acids)
RN 204267-56-1 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(3,4-dimethoxyphenyl)ethoxy]- (9CI) (CA INDEX NAME)



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

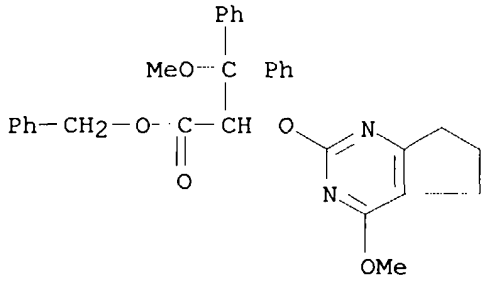
L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:635651 CAPLUS
DN 129:275935
TI Novel pyrimidine- and triazine-containing carboxylic acid derivatives, their preparation, and use as endothelin receptor antagonists in treating cancer
IN Romerdahl, Cynthia A.
PA BASF A.-G., Germany
SO PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9841206	A1	19980924	WO 1998-US4596	19980309
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6030975	A	20000229	US 1997-818622	19970314
	AU 9866946	A1	19981012	AU 1998-66946	19980309
	AU 744019	B2	20020214		
	EP 969841	A1	20000112	EP 1998-909067	19980309
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	BR 9808263	A	20000516	BR 1998-8263	19980309
	JP 2001517220	T2	20011002	JP 1998-540573	19980309
	ZA 9802136	A	19990913	ZA 1998-2136	19980313
	NO 9904426	A	19991112	NO 1999-4426	19990913
PRAI	US 1997-818622	A	19970314		
	WO 1998-US4596	W	19980309		

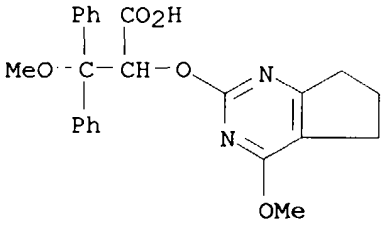
OS MARPAT 129:275935
AB The invention provides a method for treating cancer, wherein the cancer is a tumor in which endothelin (ET) is upregulated (e.g. tumors of the prostate, lung, liver, breast, brain, stomach, colon, endometrium, testicle, thyroid, pituitary, bladder, kidney, pancreas and meninges), by administering a compd. I [R = CHO, tetrazolyl, cyano, CO2H or its hydrolyzable derivs.; R2 = H, OH, (di)(alkyl)amino, halo, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio; X = N, CH, C-alkyl, or forms a 5- or 6-ring to R3; R3 = groups given for R2, or NHO-alkyl, or forms 5- or 6-ring to X; R4, R5 = (un)substituted Ph, naphthyl, or certain fused derivs.; or R4 = a wide variety of possible substituents and R5 = H, alk(en/yn)yl, cycloalkyl, haloalkyl, Ph, etc.; or R4R5 forms (un)substituted 3- to 8-ring; R6 = H, (un)substituted alk(en/yn)yl, cycloalkyl, Ph, naphthyl, heteroaryl; Y, Z = S, O, bond; with provisos]. Over 150 compds. were prepd. For instance, methanolysis of Me 3,3-diphenyl-2,3-epoxypropionate in the presence of BF3.OEt2 gave 88% Me 2-hydroxy-3-methoxy-3,3-diphenylpropionate, which was etherified with 4,6-dimethoxy-2-(methylsulfonyl)pyrimidine to give 82% title compd. II. At 150 mg/kg/day i.p. in mice in the DU-145 prostate tumor model, II reduced mean tumor wt. to 33% of control after 10 days.
IT **178306-59-7P 178306-60-0P 178306-75-7P**
178306-76-8P 178306-77-9P 213773-04-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-contg. carboxylic acid derivs. as endothelin-based anticancer agents)

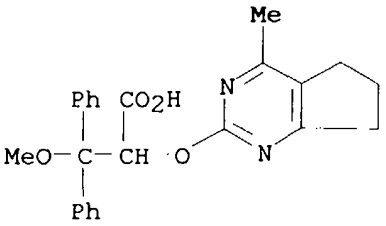
RN 178306-59-7 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 178306-60-0 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)

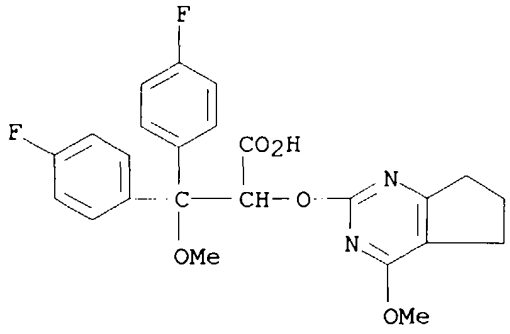


RN 178306-75-7 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methyl-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)

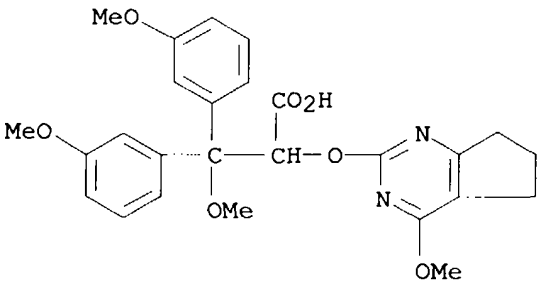


RN 178306-76-8 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-4-fluoro-.beta.-(4-fluorophenyl)-.beta.-

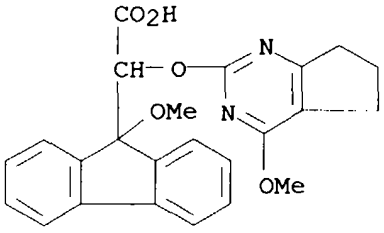
methoxy- (9CI) (CA INDEX NAME)



RN 178306-77-9 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.,3-dimethoxy-.beta.-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 213773-04-7 CAPLUS
CN 9H-Fluorene-9-acetic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-9-methoxy- (9CI) (CA INDEX NAME)



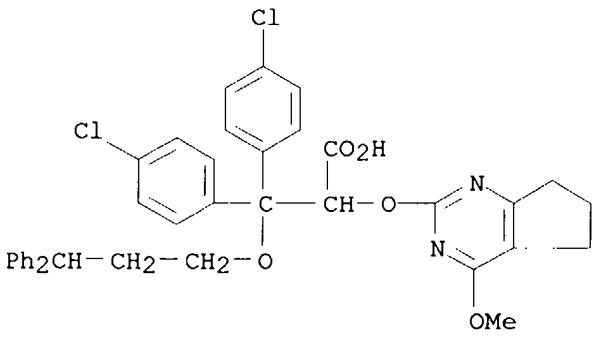
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:175913 CAPLUS
DN 128:217378
TI Preparation of .alpha.-(azinyloxy)diarylpropionates as ETA/ETB antagonists
IN Amberg, Wilhelm; Jansen, Rolf; Kling, Andreas; Klinge, Dagmar; Riechers, Hartmut; Hergenroder, Stefan; Raschack, Manfred; Unger, Liliane
PA BASF Aktiengesellschaft, Germany; Amberg, Wilhelm; Jansen, Rolf; Kling, Andreas; Klinge, Dagmar; Riechers, Hartmut; Hergenroder, Stefan; Raschack, Manfred; Unger, Liliane
SO PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

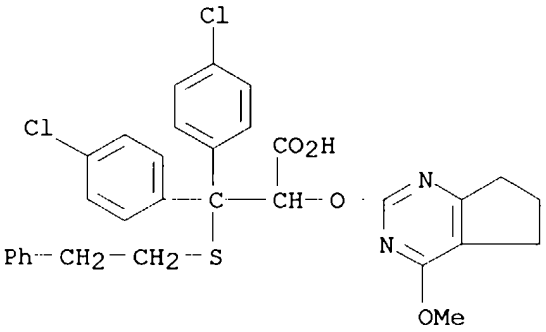
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9809953	A2	19980312	WO 1997-EP4688	19970902
	WO 9809953	A3	19981029		
	W: AL, AU, BG, BR, CA, CN, CZ, GE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19636046	A1	19980312	DE 1996-19636046	19960905
	AU 9745524	A1	19980326	AU 1997-45524	19970902
	AU 736414	B2	20010726		
	EP 929529	A2	19990721	EP 1997-943819	19970902
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, SI, FI, RO				
	BR 9711693	A	19990824	BR 1997-11693	19970902
	CN 1236362	A	19991124	CN 1997-199458	19970902
	JP 2000517329	T2	20001226	JP 1998-512203	19970902
	ZA 9707946	A	19990304	ZA 1997-7946	19970904
	NO 9901079	A	19990504	NO 1999-1079	19990304
	BG 103258	A	20001229	BG 1999-103258	19990316
PRAI	DE 1996-19636046	A	19960905		
	WO 1997-EP4688	W	19970902		

OS MARPAT 128:217378
AB R6QWCR4R5CH(OR)R1 [I; Q = C2-4 spacer (sic); R = cyclic group II; R1 = CO2R7, CONHSO2R9, CONR13R14, etc.; R2,R3 = H, halo, alkyl, alkoxy, etc.; R4,R5 = (un)substituted Ph, -naphthyl, -biphenylyl, etc.; R6 = cycloalkyl, Ph, heteroaryl, etc.; R7 = H, alkyl, phenyl(methyl), etc.; R9 = alk(en)yl, phenyl(alkyl), etc.; R13,R14 = H, alkyl, Ph, CH2Ph, etc.; W = O or S; X,Y = N or CH; Z = N, (un)substituted CH, etc.] were prepd. Thus, (4-EtC6H4)2CO was cyclocondensed with ClCH2CO2Me and the resulting epoxide condensed with 3,4-(MeO)2C6H3CH2CH2OH to give 3,4-(MeO)2C6H3CH2CH2OC(C6H4Et-4)2CH(OH)CO2Me which was sapond. and the product etherified by 4-methoxy-6-methyl-2-methylsulfonylpyrimidine to give title compd. III. Data for biol. activity of I were given.
IT **204267-51-6P 204267-52-7P 204267-53-8P**
204267-54-9P 204267-55-0P 204267-56-1P
204267-57-2P 204268-02-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of .alpha.-(azinyloxy)diarylpropionates as ETA/ETB antagonists)
RN 204267-51-6 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-(3,3-

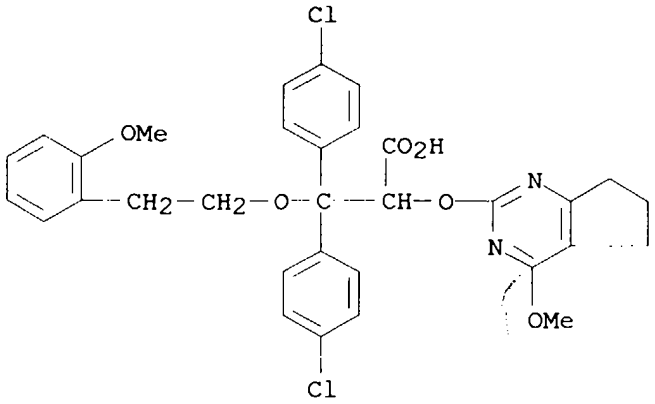
diphenylpropoxy)- (9CI) (CA INDEX NAME)



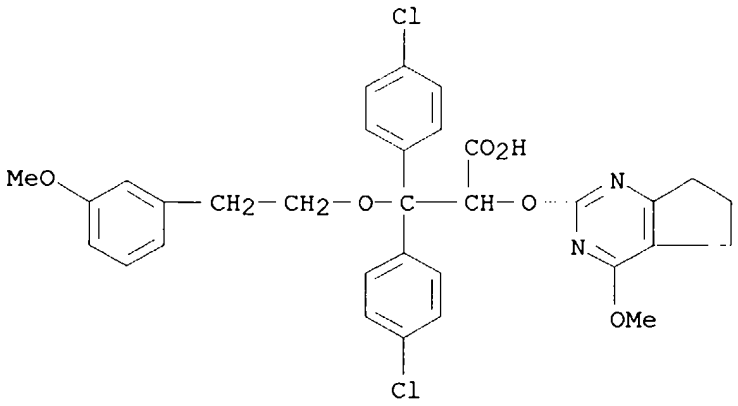
RN 204267-52-7 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[(2-phenylethyl)thio]- (9CI) (CA INDEX NAME)



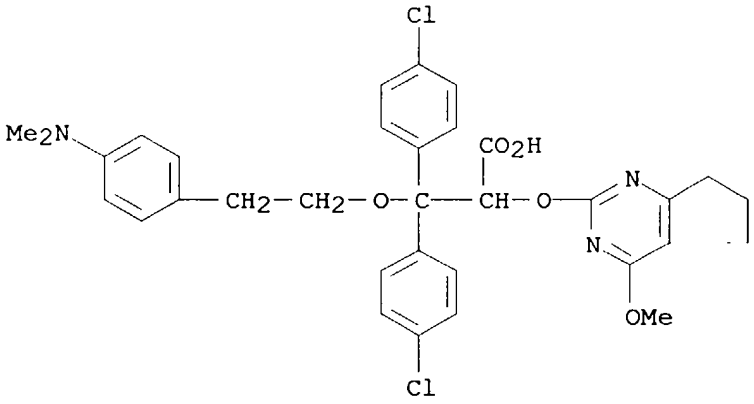
RN 204267-53-8 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(2-methoxyphenyl)ethoxy]- (9CI) (CA INDEX NAME)



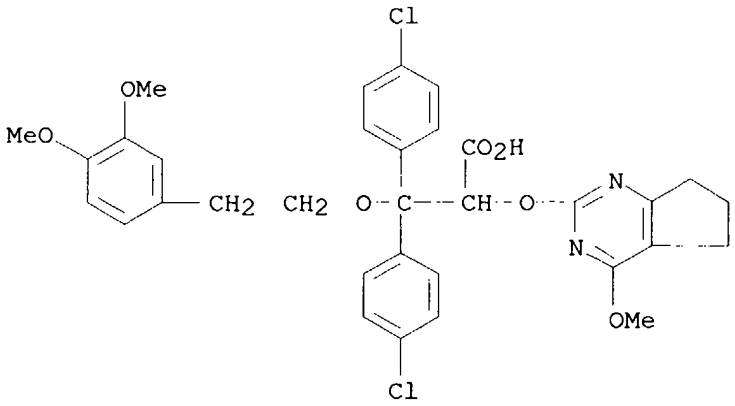
RN 204267-54-9 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(3-methoxyphenyl)ethoxy]- (9CI) (CA INDEX NAME)



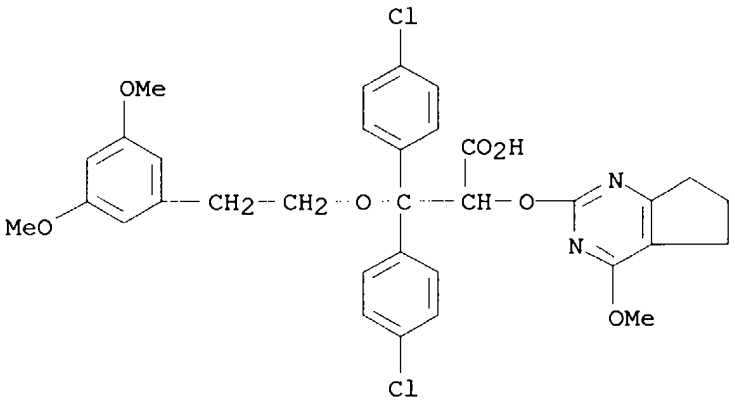
RN 204267-55-0 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-[4-(dimethylamino)phenyl]ethoxy]- (9CI) (CA INDEX NAME)



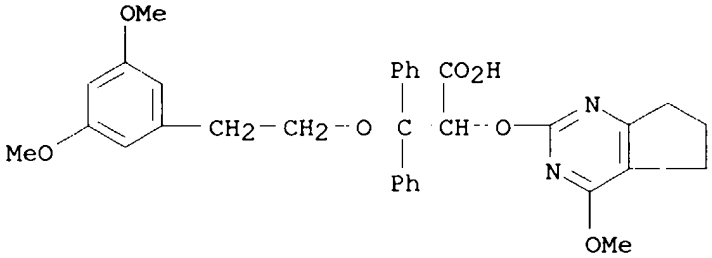
RN 204267-56-1 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(3,4-dimethoxyphenyl)ethoxy]- (9CI) (CA INDEX NAME)



RN 204267-57-2 CAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-(4-chlorophenyl)-.alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(3,5-dimethoxyphenyl)ethoxy]- (9CI) (CA INDEX NAME)



RN 204268-02-0 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-[2-(3,5-dimethoxyphenyl)ethoxy]-.beta.-phenyl- (9CI) (CA INDEX NAME)



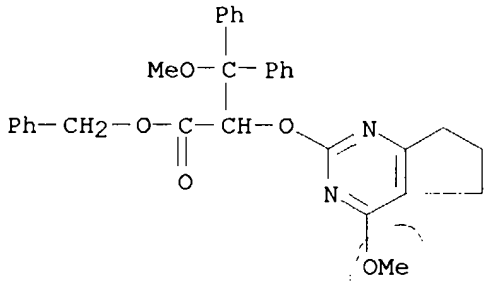
L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:401554 CAPLUS
DN 125:58534
TI Preparation of pyrimidine- and triazine-derivative endothelin receptor antagonists
IN Riechers, Hartmut; Klinge, Dagmar; Amberg, Wilhelm; Kling, Andreas; Mueller, Stefan; Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Wernet, Wolfgang; et al.
PA BASF A.-G., Germany
SO Ger. Offen., 28 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19533023	A1	19960418	DE 1995-19533023	19950907
	WO 9611914	A1	19960425	WO 1995-EP3963	19951007
	W: AU, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, MX, NO, NZ, PL, RU, SG, SI, SK, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9538045	A1	19960506	AU 1995-38045	19951007
	AU 688611	B2	19980312		
	EP 785926	A1	19970730	EP 1995-935916	19951007
	EP 785926	B1	20010822		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	CN 1160396	A	19970924	CN 1995-195655	19951007
	BR 9509338	A	19971104	BR 1995-9338	19951007
	HU 77443	A2	19980428	HU 1997-1975	19951007
	JP 10507190	T2	19980714	JP 1995-512911	19951007
	EP 1110952	A1	20010627	EP 2001-103889	19951007
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	AT 204568	E	20010915	AT 1995-935916	19951007
	ES 2162942	T3	20020116	ES 1995-935916	19951007
	RU 2180335	C2	20020310	RU 1997-107617	19951007
	ZA 9508642	A	19970414	ZA 1995-8642	19951013
	US 5932730	A	19990803	US 1997-809699	19970327
	FI 9701529	A	19970411	FI 1997-1529	19970411
	NO 9701675	A	19970610	NO 1997-1675	19970411
	US 5969134	A	19991019	US 1998-184152	19981102
	US 6197958	B1	20010306	US 1999-309770	19990511
	US 2002052495	A1	20020502	US 2000-748184	20001227
	US 6600043	B2	20030729		
PRAI	DE 1994-4436851	A1	19941014		
	DE 1995-19533023	A	19950907		
	EP 1995-935916	A3	19951007		
	WO 1995-EP3963	W	19951007		
	US 1998-184152	A3	19981102		
	US 1999-309770	A3	19990511		

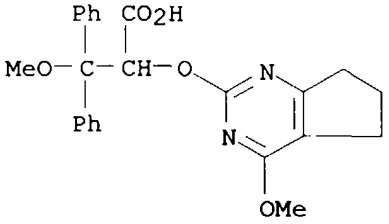
OS MARPAT 125:58534
AB The title compds. [I; R = CHO, tetrazolyl, CN, CO2H, groups cleavable to CO2H; R2 = (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R3 = H, OH, (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R4, R5 = (un)substituted Ph or naphthyl; R6 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, (un)substituted Ph, etc.; X = N, (un)substituted CH; Y = direct bond, S, O; Z = S, O, SO, SO2, direct bond], useful as endothelin receptor antagonists, are prepd. Thus, pyrimidine deriv. II, m.p. 167.degree., demonstrated a Ki ETA of 6 nM.

IT **178306-59-7P 178306-60-0P 178306-75-7P**
178306-76-8P 178306-77-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

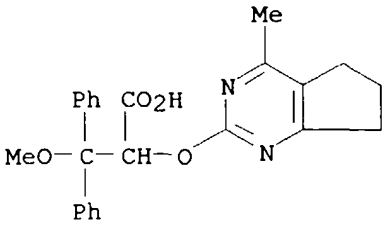
RN 178306-59-7 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 178306-60-0 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)

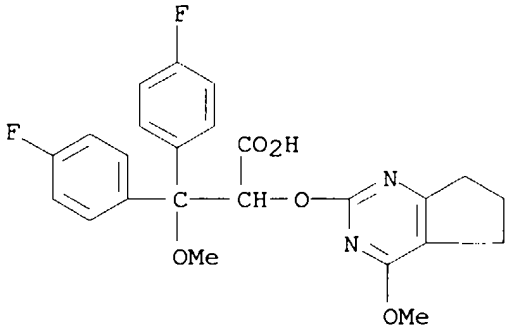


RN 178306-75-7 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methyl-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl- (9CI) (CA INDEX NAME)

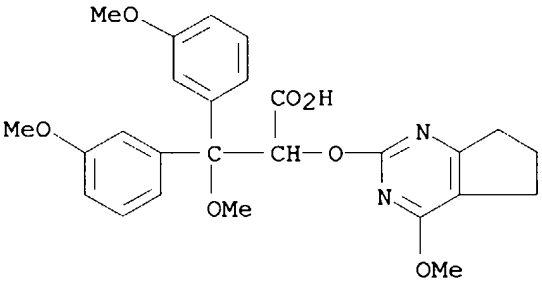


RN 178306-76-8 CAPLUS

CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-4-fluoro-.beta.-(4-fluorophenyl)-.beta.-methoxy- (9CI) (CA INDEX NAME)

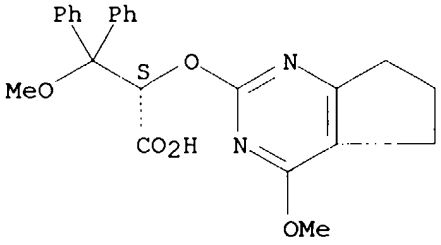


RN 178306-77-9 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.,3-dimethoxy-.beta.-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:271791 CAPLUS
DN 125:328
TI Discovery and Optimization of a Novel Class of Orally Active Nonpeptidic Endothelin-A Receptor Antagonists
AU Riechers, Hartmut; Albrecht, Hans-Peter; Amberg, Willi; Baumann, Ernst; Bernard, Harald; Boehm, Hans-Joachim; Klinge, Dagmar; Kling, Andreas; Mueller, Stefan; et al.
CS Hauptlaboratorium, BASF AG, Ludwigshafen, 67056, Germany
SO Journal of Medicinal Chemistry (1996), 39(11), 2123-8
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 125:328
AB A novel class of endothelin-A receptor ligands was discovered by high-throughput screening. Lead structure optimization led to highly potent antagonists which can be synthesized in a short sequence. The compds. are endothelin-A-selective, are orally available, and show a long duration of action.
IT **177036-96-3P**, LU 136181
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)
RN 177036-96-3 CAPLUS
CN Benzenepropanoic acid, .alpha.-[(6,7-dihydro-4-methoxy-5H-cyclopentapyrimidin-2-yl)oxy]-.beta.-methoxy-.beta.-phenyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> d his

     (FILE 'HOME' ENTERED AT 10:13:34 ON 01 DEC 2003)

     FILE 'REGISTRY' ENTERED AT 10:13:39 ON 01 DEC 2003
L1              STRUCTURE UPLOADED
L2            0 S L1 SSS SAM
L3           17 S L1 SSS FUL

     FILE 'CAPLUS' ENTERED AT 10:14:24 ON 01 DEC 2003
L4            6 S L3

     FILE 'CAOLD' ENTERED AT 10:14:55 ON 01 DEC 2003

=> s l3
L5            0 L3

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.40     176.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -3.91

STN INTERNATIONAL LOGOFF AT 10:15:08 ON 01 DEC 2003
```